

A UNIFYING FRAMEWORK FOR THE DERIVATION AND ANALYSIS OF EFFECTIVE CLASSES OF ONE-STEP METHODS FOR ODES *

LUIGI BRUGNANO[†], FELICE IAVERNARO[‡], AND DONATO TRIGIANTE[§]

Abstract. In this paper, we provide a simple framework to derive and analyse several classes of effective one-step methods. The framework consists in the discretization of a local Fourier expansion of the continuous problem. Different choices of the basis lead to different classes of methods, even though we shall here consider only the case of an orthonormal polynomial basis, from which a large subclass of Runge-Kutta methods can be derived. The obtained results are then applied to prove, in a simplified way, the order and stability properties of Hamiltonian BVMs (HBVMs), a recently introduced class of energy preserving methods for canonical Hamiltonian systems (see [1] and references therein). A few numerical tests with such methods are also included, in order to confirm the effectiveness of the methods.

Key words. Ordinary differential equations, Runge-Kutta methods, one-step methods, Hamiltonian problems, Hamiltonian Boundary Value Methods, energy preserving methods, symplectic methods, energy drift.

AMS subject classifications. 65L05, 65P10.

1. Introduction.

Though I have not always been able to make simple a difficult thing, I never made difficult a simple one.
F. G. Tricomi

One-step methods are widely used in the numerical solution of initial value problems for ordinary differential equations which, without loss of generality, we shall assume to be in the form:

$$y'(t) = f(y(t)), \quad t \in [t_0, t_0 + T], \quad y(t_0) = y_0 \in \mathbb{R}^m. \quad (1.1)$$

In particular, we consider a very general class of effective one-step methods that can be led back to a local Fourier expansion of the continuous problem over the interval $[t_0, t_0 + h]$, where h is the considered stepsize. In general, different choices of the basis result in different classes of methods, for which, however, the analysis turns out to be remarkably simple. Though the arguments can be extended to a general choice of the basis, we consider here only the case of a polynomial basis, from which one obtains a large subclass of Runge-Kutta methods. Usually, the order properties of such methods are studied through the classical theory of Butcher on rooted trees (see, e.g., [9, Th. 2.13 on p. 153]), almost always resorting to the so called *simplifying assumptions* (see, e.g., [9, Th. 7.4 on p. 208]). Nonetheless, such analysis turns out to be greatly simplified for the methods derived in the new framework, which is introduced in Section 2. Similar arguments apply to the linear stability analysis of the methods, here easily discussed through the Lyapunov method. Then, we apply the same procedure to the case where (1.1) is a canonical Hamiltonian problem, i.e., a problem in the form

$$\frac{dy}{dt} = J \nabla H(y), \quad J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix}, \quad y(t_0) = y_0 \in \mathbb{R}^{2m}, \quad (1.2)$$

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[†]Dipartimento di Matematica “U.Dini”, Università di Firenze, Italy (luigi.brugnano@unifi.it).

[‡]Dipartimento di Matematica, Università di Bari, Italy (felix@dm.uniba.it).

[§]Dipartimento di Energetica “S.Stecco”, Università di Firenze, Italy (trigiant@unifi.it).

where $H(y)$ is a smooth scalar function, thus obtaining, in Section 3, an alternative derivation of the recently introduced class of energy preserving methods called Hamiltonian BVMs (HBVMs, see [1, 2, 3] and references therein). A few numerical examples concerning such methods are then provided in Section 4, in order to make evident their potentialities. Some concluding remarks are then given in Section 5.

2. Local Fourier expansion of ODEs. Let us consider problem (1.1) restricted to the interval $[t_0, t_0 + h]$:

$$y' = f(y), \quad t \in [t_0, t_0 + h], \quad y(t_0) = y_0. \quad (2.1)$$

In order to make the arguments as simple as possible, we shall hereafter assume f to be analytical. Then, let us fix an orthonormal basis $\{\hat{P}_j\}_{j=0}^{\infty}$ over the interval $[0, 1]$, even though different bases and/or reference intervals could be in principle considered. In particular, hereafter we shall consider a polynomial basis: i.e., the shifted Legendre polynomials over the interval $[0, 1]$, scaled in order to be orthonormal. Consequently,

$$\int_0^1 \hat{P}_i(x) \hat{P}_j(x) dx = \delta_{ij}, \quad \deg \hat{P}_j = j, \quad \forall i, j \geq 0,$$

where δ_{ij} is the Kronecker symbol. We can then rewrite (2.1) by expanding the right-hand side:

$$y'(t_0 + ch) = \sum_{j=0}^{\infty} \hat{P}_j(c) \gamma_j(y), \quad c \in [0, 1]; \quad \gamma_j(y) = \int_0^1 \hat{P}_j(\tau) f(y(t_0 + \tau h)) d\tau. \quad (2.2)$$

The basic idea (first sketched in [5]) is now that of truncating the series iafter r terms, which turns (2.2) into

$$\omega'(t_0 + ch) = \sum_{j=0}^{r-1} \hat{P}_j(c) \gamma_j(\omega), \quad c \in [0, 1]; \quad \gamma_j(\omega) = \int_0^1 \hat{P}_j(\tau) f(\omega(t_0 + \tau h)) d\tau. \quad (2.3)$$

By imposing the initial condition, one then obtains

$$\omega(t_0 + ch) = y_0 + h \sum_{j=0}^{r-1} \gamma_j(\omega) \int_0^c \hat{P}_j(x) dx, \quad c \in [0, 1]. \quad (2.4)$$

Obviously, ω is a polynomial of degree at most r . The following question then naturally arises: “how close are $y(t_0 + h)$ and $\omega(t_0 + h)$?” The answer is readily obtained, by using the following preliminary result.

LEMMA 2.1. *Let $g : [0, h] \rightarrow \mathbb{R}^m$ be a suitably regular function. Then $\int_0^1 \hat{P}_j(\tau) g(\tau h) d\tau = O(h^j)$.*

Proof. Assume, for sake of simplicity,

$$g(\tau h) = \sum_{n=0}^{\infty} \frac{g^{(n)}(0)}{n!} (\tau h)^n$$

to be the Taylor expansion of g . Then, for all $j \geq 0$,

$$\int_0^1 \hat{P}_j(\tau) g(\tau h) d\tau = \sum_{n=0}^{\infty} \frac{g^{(n)}(0)}{n!} h^n \int_0^1 \hat{P}_j(\tau) \tau^n d\tau = O(h^j),$$

since \hat{P}_j is orthogonal to polynomials of degree $n < j$. \square

As a consequence, one has that (see (2.3)) $\gamma_j(\omega) = O(h^j)$. Moreover, for any given $\tilde{t} \in [t_0, t_0 + h]$, we denote by $y(s, \tilde{t}, \tilde{y})$ the solution of (2.1)-(2.2) at time s and with initial condition $y(\tilde{t}) = \tilde{y}$. Similarly, we denote by

$$\Phi(s, \tilde{t}, \tilde{y}) = \frac{\partial}{\partial \tilde{y}} y(s, \tilde{t}, \tilde{y}), \quad (2.5)$$

also recalling the following standard result from the theory of ODEs:

$$\frac{\partial}{\partial \tilde{t}} y(s, \tilde{t}, \tilde{y}) = -\Phi(s, \tilde{t}, \tilde{y}) f(\tilde{y}). \quad (2.6)$$

We can now state the following result, for which we provide a more direct proof, with respect to that given in [5]. Such proof is essentially based on that of [12, Theorem 6.5.1 on pp. 165-166].

THEOREM 2.2. *Let $y(t_0 + ch)$ and $\omega(t_0 + ch)$, $c \in [0, 1]$, be the solutions of (2.2) and (2.3), respectively. Then, $y(t_0 + h) - \omega(t_0 + h) = O(h^{2r+1})$.*

Proof. By virtue of Lemma 2.1 and (2.5)-(2.6), one has:

$$\begin{aligned} y(t_0 + h) - \omega(t_0 + h) &= y(t_0 + h, t_0, y_0) - y(t_0 + h, t_0 + h, \omega(t_0 + h)) \\ &= \int_{t_0}^{t_0+h} \frac{d}{d\tau} y(t_0 + h, \tau, \omega(\tau)) d\tau = \int_{t_0}^{t_0+h} \left(\frac{\partial}{\partial \tau} y(t_0 + h, \tau, \omega(\tau)) + \frac{\partial}{\partial \omega} y(t_0 + h, \tau, \omega(\tau)) \omega'(\tau) \right) d\tau \\ &= h \int_0^1 \Phi(t_0 + h, t_0 + ch, \omega(t_0 + ch)) (-f(\omega(t_0 + ch)) + \omega'(t_0 + ch)) dc \\ &= -h \int_0^1 \Phi(t_0 + h, t_0 + ch, \omega(t_0 + ch)) \left(\sum_{j=r}^{\infty} \gamma_j(\omega) \hat{P}_j(c) \right) dc \\ &= -h \sum_{j=r}^{\infty} \left(\int_0^1 \hat{P}_j(\tau) \Phi(t_0 + h, t_0 + ch, \omega(t_0 + ch)) d\tau \right) \gamma_j(\omega) = h \sum_{j=r}^{\infty} O(h^j) O(h^j) = O(h^{2r+1}). \end{aligned}$$

\square

The previous result reveals the extent to which the polynomial $\omega(t)$, solution of (2.3), approximates the solution $y(t)$ of the original problem (2.1) on the time interval $[t_0, t_0 + h]$. Obviously, the value $\omega(t_0 + h)$ may serve as the initial condition for a new IVP in the form (2.3) approximating $y(t)$ on the time interval $[t_0 + h, t_0 + 2h]$. In general, setting $t_i = t_0 + ih$, $i = 0, 1, \dots$, and assuming that an approximation $\omega(t)$ is available on the interval $[t_{i-2}, t_{i-1}]$, one can extend the approximation to the interval $[t_{i-1}, t_i]$ by solving the IVP

$$\omega'(t_{i-1} + ch) = \sum_{j=0}^{r-1} \hat{P}_j(c) \int_0^1 \hat{P}_j(\tau) f(\omega(t_{i-1} + ch)) d\tau, \quad c \in [0, 1], \quad (2.7)$$

the initial value $\omega(t_{i-1})$ having been computed at the preceding step. The approximation to $y(t)$ is thus extended on an arbitrary interval $[t_0, t_0 + Nh]$, and the function $\omega(t)$ is a continuous piecewise polynomial. As a direct consequence of Theorem 2.2, we obtain the following result.

COROLLARY 1. *Let $T = Nh$, where $h > 0$ and N is an integer. Then, the approximation to the solution of problem (1.1) by means of (2.7) at the grid-points $t_i = t_{i-1} + h$, $i = 1, \dots, N$, with $\omega(t_0) = y_0$, is $O(h^{2r})$ accurate.*

We now want to compare the asymptotic behavior of $\omega(t)$ and $y(t)$ on the infinite length interval $[t_0, +\infty)$ in the case where f is linear or defines a canonical Hamiltonian problem. To this end we introduce the infinite sequence $\{\omega_i\} \equiv \{\omega(t_i)\}$.

REMARK 1. *Though in general, the sequence $\{\omega_i\}$ cannot be formally regarded as the outcome of a numerical method, under special situations, this can be the case. For example, when f is a polynomial, the integrals in (2.3) may be explicitly determined and the IVP in (2.3) is evidently equivalent to a nonlinear system having as unknowns the coefficients of the polynomial ω expanded along a given basis (for example, the polynomial ω may be computed by means of the method of undetermined coefficients). This issue, as well as details about how to manage the integrals in the event that the integrands do not admit an analytical primitive function in closed form, will be thoroughly faced in Section 3.*

2.1. Linear stability analysis. For the linear stability analysis, problem (2.1) becomes the celebrated test equation

$$y' = \lambda y, \quad \Re(\lambda) \leq 0. \quad (2.8)$$

By setting

$$\lambda = \alpha + i\beta, \quad y = x_1 + ix_2, \quad x = (x_1, x_2)^T, \quad A = \begin{pmatrix} \alpha & -\beta \\ \beta & \alpha \end{pmatrix},$$

with i the imaginary unit, problem (2.8) can be rewritten as

$$x' = Ax, \quad t \in [t_0, t_0 + h], \quad x(t_0) \text{ given.} \quad (2.9)$$

Consequently, the corresponding truncated problem (2.3) becomes

$$\omega'(t_0 + ch) = A \sum_{j=0}^{r-1} \hat{P}_j(c) \int_0^1 \hat{P}_j(\tau) \nabla V(\omega(t_0 + \tau h)) d\tau, \quad c \in [0, 1], \quad (2.10)$$

where

$$V(x) = \frac{1}{2} x^T x \quad (2.11)$$

is a Lyapunov function for (2.9). From (2.10)-(2.11) one readily obtains

$$\begin{aligned} \Delta V(\omega(t_0)) &= V(\omega(t_0 + h)) - V(\omega(t_0)) = h \int_0^1 \nabla V(\omega(t_0 + \tau h))^T \omega'(t_0 + \tau h) d\tau \\ &= h \sum_{j=0}^{r-1} \left[\int_0^1 \hat{P}_j(\tau) \nabla V(\omega(t_0 + \tau h)) d\tau \right]^T A \left[\int_0^1 \hat{P}_j(\tau) \nabla V(\omega(t_0 + \tau h)) d\tau \right] \\ &= \alpha h \sum_{j=0}^{r-1} \left\| \int_0^1 \hat{P}_j(\tau) \omega(t_0 + \tau h) d\tau \right\|_2^2. \end{aligned}$$

Last equality follows by taking the symmetric part of A . We observe that

$$\omega \neq 0 \implies \sum_{j=0}^{r-1} \left\| \int_0^1 \hat{P}_j(\tau) \omega(t_0 + \tau h) d\tau \right\|_2^2 > 0,$$

since, conversely, this would imply $\omega(t_0 + ch) = \rho \cdot \hat{P}_r(c)$ for a suitable $\rho \neq 0$ and, therefore (from (2.10)), $\hat{P}'_r \equiv 0$ which is clearly not true. Thus for a generic $y_0 \neq 0$,

$$\Delta V(\omega(t_0)) < 0 \iff \Re(\lambda) < 0 \quad \text{and} \quad \Delta V(\omega(t_0)) = 0 \iff \Re(\lambda) = 0.$$

Again, the above computation can be extended to any interval $[t_{i-1}, t_i]$ and, from the discrete version of the Lyapunov theorem (see, e.g., [12, Th. 4.8.3 on p. 108]), we have that the sequence ω_i tends to zero if and only if $\Re(\lambda) < 0$, while it remains bounded whenever $\Re(\lambda) = 0$, whatever is the stepsize $h > 0$ used. The following result is thus proved.

THEOREM 2.3. *The continuous solution $y(t)$ of (2.8) and its discrete approximation ω_i have the same stability properies, for any choice of the stepsize $h > 0$.*

2.2. The Hamiltonian case. In the case where problem (1.1) is Hamiltonian, i.e., (1.2), the approximation provided by the polynomial ω in (2.3)-(2.4) inherits a very important property of the continuous problem, i.e., energy conservation. Indeed, it is very well known that for the continuous solution one has, by virtue of (1.2),

$$\frac{d}{dt}H(y(t)) = \nabla H(y(t))^T y'(t) = \nabla H(y(t))^T J \nabla H(y(t)) = 0,$$

due to the fact that matrix J is skew-symmetric. Consequently, $H(y(t)) = H(y_0)$ for all t . For the truncated Fourier problem, the following result holds true.

THEOREM 2.4. $H(\omega(t_0 + h)) = H(\omega(t_0)) \equiv H(y_0)$.

Proof. From (2.3), considering that $f(\omega) = J \nabla H(\omega)$ and $J^T J = I$, one obtains:

$$\begin{aligned} H(\omega(t_0 + h)) - H(y_0) &= \\ &= h \int_0^1 \nabla H(\omega(t_0 + \tau h))^T \omega'(t_0 + \tau h) d\tau = h \int_0^1 \nabla H(\omega(t_0 + \tau h))^T \sum_{j=0}^{r-1} \hat{P}_j(\tau) \gamma_j(\omega) d\tau \\ &= h \sum_{j=0}^{r-1} \left(\int_0^1 \nabla H(\omega(t_0 + \tau h)) \hat{P}_j(\tau) d\tau \right)^T \gamma_j(\omega) = h \sum_{j=0}^{r-1} \gamma_j(\omega)^T J \gamma_j(\omega) = 0, \end{aligned}$$

since J is skew-symmetric. \square

3. Discretization. Clearly, the integrals in (2.3), if not directly computable, need to be numerically approximated. This can be done by introducing a quadrature formula based at $k \geq r$ abscissae $\{c_i\}$, thus obtaining an approximation to (2.3):

$$u'(t_0 + ch) = \sum_{j=0}^{r-1} \hat{P}_j(c) \sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) f(u(t_0 + c_\ell h)), \quad c \in [0, 1]. \quad (3.1)$$

where the $\{b_\ell\}$ are the quadrature weights, and u is the resulting polynomial, of degree at most r , approximating ω . It can be obtained by solving a discrete problem in the form:

$$u'(t_0 + c_i h) = \sum_{j=0}^{r-1} \hat{P}_j(c_i) \sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) f(u(t_0 + c_\ell h)), \quad i = 1, \dots, k. \quad (3.2)$$

Let q be the order of the formula, i.e., let it be exact for polynomials of degree less than q (we observe that $q \geq k \geq r$). Clearly, since we assume f to be analytical, choosing k large enough, along with a suitable choice of the nodes $\{c_i\}$, allows to approximate the given integral to any degree of accuracy, even though, when using finite precision arithmetic, it suffices to approximate it to machine precision. We observe that, since the quadrature is exact for polynomials of degree $q - 1$, then its remainder depends on the q -th derivative of the integrand with respect to τ . Consequently, considering that $\hat{P}_j^{(i)}(c) \equiv 0$, for $i > j$, one has

$$\Delta_j(h) \equiv \int_0^1 \hat{P}_j(\tau) f(u(t_0 + \tau h)) d\tau - \sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) f(u(t_0 + c_\ell h)) = O(h^{q-j}), \quad (3.3)$$

$j = 0, \dots, r-1$. Thus, (3.1) is equivalent to the ODE,

$$u'(t_0 + ch) = \sum_{j=0}^{r-1} \hat{P}_j(c) (\gamma_j(u) - \Delta_j(h)), \quad c \in [0, 1], \quad \gamma_j(u) = \int_0^1 \hat{P}_j(\tau) f(u(t_0 + \tau h)) d\tau, \quad (3.4)$$

with $u(t_0) = y_0$, in place of (2.3). The following result then holds true.

THEOREM 3.1. *In the above hypotheses: $y(t_0 + h) - u(t_0 + h) = O(h^{p+1})$, with $p = \min(q, 2r)$.*

Proof. The proof is quite similar to that of Theorem 2.2: by virtue of Lemma 2.1 and (3.3)-(3.4), one obtains

$$\begin{aligned} y(t_0 + h) - u(t_0 + h) &= y(t_0 + h, t_0, y_0) - y(t_0 + h, t_0 + h, u(t_0 + h)) \\ &= \int_{t_0}^{t_0+h} \frac{d}{d\tau} y(t_0 + h, \tau, u(\tau)) d\tau = \int_{t_0}^{t_0+h} \left(\frac{\partial}{\partial \tau} y(t_0 + h, \tau, u(\tau)) + \frac{\partial}{\partial u} y(t_0 + h, \tau, u(\tau)) u'(\tau) \right) d\tau \\ &= h \int_0^1 \Phi(t_0 + h, t_0 + ch, u(t_0 + ch)) (-f(u(t_0 + ch)) + u'(t_0 + ch)) dc \\ &= h \int_0^1 \Phi(t_0 + h, t_0 + ch, u(t_0 + ch)) \left(\sum_{j=0}^{r-1} \hat{P}_j(c) \Delta_j(h) - \sum_{j=r}^{\infty} \gamma_j(u) \hat{P}_j(c) \right) dc \\ &= h \sum_{j=0}^{r-1} \left(\int_0^1 \hat{P}_j(\tau) \Phi(t_0 + h, t_0 + ch, u(t_0 + ch)) d\tau \right) \Delta_j(u) \\ &\quad - h \sum_{j=r}^{\infty} \left(\int_0^1 \hat{P}_j(\tau) \Phi(t_0 + h, t_0 + ch, u(t_0 + ch)) d\tau \right) \gamma_j(u) \\ &= h \sum_{j=0}^{r-1} O(h^j) O(h^{q-j}) - h \sum_{j=r}^{\infty} O(h^j) O(h^j) = O(h^{q+1}) + O(h^{2r+1}). \end{aligned}$$

□

As an immediate consequence, one has the following result.

COROLLARY 2. *Let q be the order of the quadrature formula defined by the abscissae $\{c_i\}$. Then, the order of the method (3.2) for approximating (1.1), with $y_1 = u(t_0 + h)$, is $p = \min(q, 2r)$.*

Concerning the linear stability analysis, by considering that a quadrature formula of order $q \geq 2r$

is exact when the integrand is a polynomial of degree at most $2r - 1$, the following result immediately derives from Theorem 2.3.

COROLLARY 3. *Let q be the order of the quadrature formula defined by the abscissae $\{c_i\}$. If $q \geq 2r$, then the method (3.2) is perfectly A-stable.¹*

In the case $r = 1$, the above results apply to the methods in [10] (see also [11]).

3.1. Runge-Kutta formulation. By setting, as usual, $u_i = u(t_0 + c_i h)$, $f_i = f(u_i)$, $i = 1, \dots, k$, (3.2) can be rewritten as

$$u_i = y_0 + h \sum_{j=0}^{r-1} \int_0^{c_i} \hat{P}_j(\tau) d\tau \sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) f_\ell, \quad i = 1, \dots, k. \quad (3.5)$$

Moreover, since $q \geq r \geq \deg u$, one has $y_1 = u(t_0 + h) \equiv y_0 + h \sum_{\ell=1}^k b_\ell f_\ell$. Consequently, the methods which Corollary 2 refers to are the subclass of Runge-Kutta methods with the following tableau:

$$\begin{array}{c|c} \begin{array}{c} c_1 \\ \vdots \\ c_k \end{array} & A = (a_{ij}) \equiv \left(b_j \sum_{\ell=0}^{r-1} \hat{P}_\ell(c_j) \int_0^{c_i} \hat{P}_\ell(\tau) d\tau \right) \\ \hline & \begin{array}{ccc} b_1 & \dots & b_k \end{array} \end{array} \quad (3.6)$$

In particular, in [4] it has been proved that when the nodes $\{c_i\}$ coincide with the k Gauss points in the interval $[0, 1]$, then

$$A = \mathcal{A} \mathcal{P} \mathcal{P}^T \Omega,$$

where $\mathcal{A} \in \mathbb{R}^{k \times k}$ is the matrix in the Butcher tableau of the k -stages Gauss method, $\mathcal{P} = (\hat{P}_{j-1}(c_i)) \in \mathbb{R}^{k \times r}$, and $\Omega = \text{diag}(b_1, \dots, b_k)$. In such a way, when $k = r$, one obtains the classical r -stages Gauss collocation method. Consequently, (3.6) can be regarded as a generalization of the classical Runge-Kutta collocation methods, (3.2) being interpreted as *extended collocation conditions*.

3.2. Hamiltonian Boundary Value Methods (HBVMs). When considering a canonical Hamiltonian problem (1.2), the discretization of the integrals appearing in (2.3) by means of a Gaussian formula at k nodes results in the HBVM(k, r) methods introduced in [3].² For such methods we derive, in a novel way with respect to [1, 2, 3], the following result.

COROLLARY 4. *For all $k \geq r$, HBVM(k, r) is perfectly A-stable and has order $2r$. The method is energy conserving for all polynomial Hamiltonians of degree not larger than $2k/r$.*

¹I.e., its absolute stability region coincides with the left-half complex plane, \mathbb{C}^- , [6].

²A different discretization, based at $k + 1$ Lobatto abscissae, was previously considered in [2].

Proof. The result on the order and linear stability easily follow from Corollaries 2 and 3, respectively. Concerning energy conservation, one has

$$\begin{aligned}
H(u(t_0 + h)) - H(y_0) &= h \int_0^1 \nabla H(u(t_0 + \tau h))^T u'(t_0 + \tau h) d\tau \\
&= h \int_0^1 \nabla H(u(t_0 + \tau h))^T \sum_{j=0}^{r-1} \hat{P}_j(\tau) \sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) J \nabla H(u(t_0 + c_\ell h)) d\tau \\
&= h \sum_{j=0}^{r-1} \left[\int_0^1 \hat{P}_j(\tau) \nabla H(u(t_0 + \tau h)) d\tau \right]^T J \left[\sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) \nabla H(u(t_0 + c_\ell h)) \right] = 0,
\end{aligned}$$

provided that

$$\int_0^1 \hat{P}_j(\tau) \nabla H(u(t_0 + \tau h)) d\tau = \sum_{\ell=1}^k b_\ell \hat{P}_j(c_\ell) \nabla H(u(t_0 + c_\ell h)). \quad (3.7)$$

In the case where H is a polynomial of degree ν , this is true provided that the integrand is a polynomial of degree at most $2k - 1$. Consequently, $\nu r - 1 \leq 2k - 1$, i.e., $\nu \leq 2k/r$. \square

In the case of general Hamiltonian problems, if we consider the limit as $k \rightarrow \infty$ we recover formulae (2.3), which have been called *HBVM*(∞, r) (or, more in general, ∞ -*HBVMs*) [1, 3]: by the way, (2.4) is nothing but the *Master Functional Equation* in [1, 3]. In the particular case $r = 1$, we derive the *averaged vector field* in [14] (for a related approach see [7]).

REMARK 2. We observe that, in the case of polynomial Hamiltonian systems, if (3.7) holds true for $k = k^*$, then

$$\text{HBVM}(k, r) \equiv \text{HBVM}(k^*, r) \equiv \text{HBVM}(\infty, r), \quad \forall k \geq k^*.$$

That is, (3.1) coincides with (2.3), for all $k \geq k^*$. In the non polynomial case, the previous conclusions continue “practically” to hold, provided that the integrals are approximated within machine precision.

REMARK 3. As is easily deduced from the arguments in Section 3.1, the *HBVM*(r, r) method is nothing but the r -stages Gauss method of order $2r$ (see also [3]).

4. Numerical Tests. We here provide a few numerical tests, showing the effectiveness of HBVMs, namely of the methods obtained in the new framework, when the problem (1.1) is in the form (1.2). In particular, we consider the Kepler problem, whose Hamiltonian is (see, e.g., [8, p. 9]):

$$H([q_1, q_2, p_1, p_2]^T) = \frac{1}{2} (p_1^2 + p_2^2) - (q_1^2 + q_2^2)^{-\frac{1}{2}}.$$

When started at

$$\begin{pmatrix} 1 - e, & 0, & 0, & \sqrt{(1+e)/(1-e)} \end{pmatrix}^T, \quad e \in [0, 1),$$

it has an elliptic periodic orbit of period 2π and eccentricity e . When e is close to 0, the problem is efficiently solved by using a constant stepsize. However, it becomes more and more difficult as $e \rightarrow 1$, so that a variable-step integration would be more appropriate in this case. We now compare the following 6-th order methods for solving such problem over a 1000 periods interval:

- HBVM(3,3), i.e., the GAUSS6 method, which is a symmetric and symplectic method;

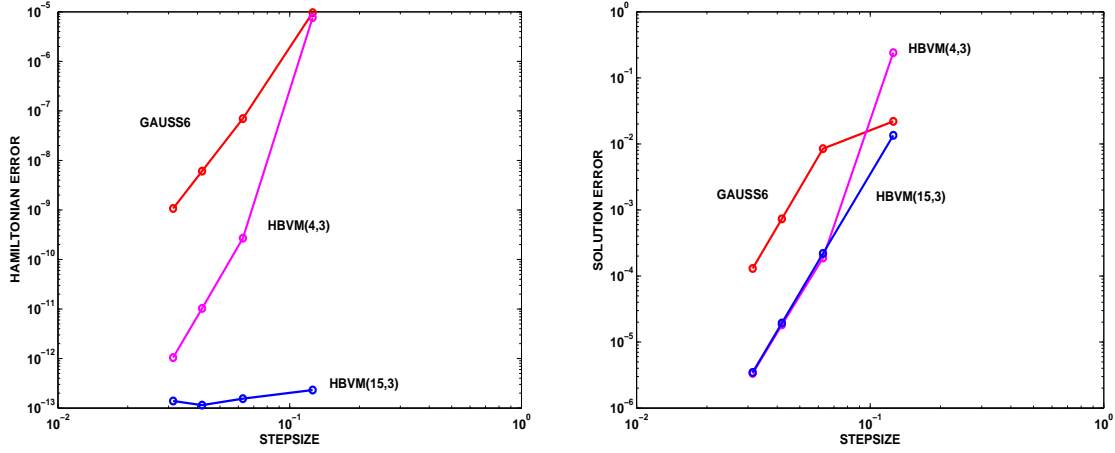


FIG. 4.1. Kepler problem, $e = 0.6$, Hamiltonian (left plot) and solution (right plot) errors over 1000 periods with a constant stepsize.

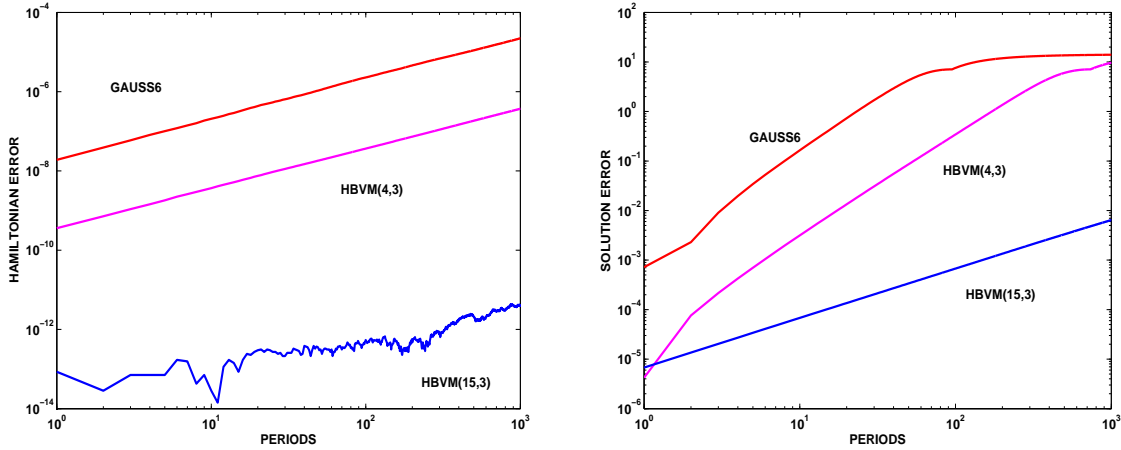


FIG. 4.2. Kepler problem, $e = 0.99$, Hamiltonian (left plot) and solution (right plot) errors over 1000 periods with a variable stepsize, $Tol = 10^{-10}$. Note that HBVM(4,3) is not energy preserving, on the contrary of HBVM(15,3).

- HBVM(4,3), which is symmetric [2] but not symplectic nor energy preserving, since the Gauss quadrature formula of order 8 is not enough accurate, for this problem;
- HBVM(15,3), which is *practically* energy preserving, since the Gauss formula of order 30 is accurate to machine precision, for this problem.

In the two plots in Figure 4.1 we see the obtained results when $e = 0.6$ and a constant stepsize is used: as one can see, the Hamiltonian is approximately conserved for the GAUSS6 and HBVM(4,3) methods, and (practically) exactly conserved for the HBVM(15,3) method. Moreover, all methods exhibit the same order (i.e., 6), with the error constant of the HBVM(4,3) and HBVM(15,3) methods much smaller than that of the symplectic GAUSS6 method. On the other hand, when $e = 0.99$, we

consider a variable stepsize implementation with the following *standard* mesh-selection strategy:

$$h_{new} = 0.7 \cdot h_n \left(\frac{Tol}{err_n} \right)^{1/(p+1)},$$

where $p = 6$ is the order of the method, Tol is the used tolerance, h_n is the current stepsize, and err_n is an estimate of the local error. According to what stated in the literature, see, e.g., [15, pp.125–127], [13, p.235], [8, pp.303–305], this is not an advisable choice for symplectic methods, for which a *drift* in the Hamiltonian appears, and a *quadratic* error growth is experienced, as is confirmed by the plots in Figure 4.2. The same happens for the method HBVM(4,3), which is not energy preserving. Conversely, for the (practically) energy preserving method HBVM(15,3), *no drift* in the Hamiltonian occurs and a *linear* error growth is observed.

REMARK 4. *We observe that more refined (though more involved) mesh selection strategies exist for symplectic methods aimed to avoid the numerical drift in the Hamiltonian and the quadratic error growth (see, e.g., [8, Chapter VIII]). However, we want to emphasize that they are no more necessary, when using energy preserving methods, since obviously no drift can occur, in such a case.*

5. Conclusions. In this paper, we have presented a general framework for the derivation and analysis of effective one-step methods, which is based on a local Fourier expansion of the problem at hand. In particular, when the chosen basis is a polynomial one, we obtain a large subclass of Runge-Kutta methods, which can be regarded as a generalization of Gauss collocation methods.

When dealing with canonical Hamiltonian problems, the methods coincide with the recently introduced class of energy preserving methods named HBVMs. A few numerical tests seem to show that such methods are less sensitive to a wider class of perturbations, with respect to symplectic, or symmetric but non energy conserving, methods. As matter of fact, on the contrary of the latter methods, they can be conveniently associated with standard mesh selection strategies.

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